Welcome to STN International! Enter x:x

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Web Page for STN Seminar Schedule - N. America
NEWS
NEWS
     2 AUG 15 CAOLD to be discontinued on December 31, 2008
NEWS
                EPFULL enhanced with full implementation of EPC2000
     3 OCT 07
NEWS 4 OCT 07 Multiple databases enhanced for more flexible patent
                number searching
NEWS 5 OCT 22 Current-awareness alert (SDI) setup and editing
                enhanced
NEWS 6 OCT 22 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
                Applications
NEWS
     7 OCT 24 CHEMLIST enhanced with intermediate list of
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        NOV 21 CAS patent coverage to include exemplified prophetic
NEWS 8
                substances identified in English-, French-, German-,
                and Japanese-language basic patents from 2004-present
NEWS 9
        NOV 26 MARPAT enhanced with FSORT command
NEWS 10
        NOV 26 MEDLINE year-end processing temporarily halts
                availability of new fully-indexed citations
NEWS 11 NOV 26 CHEMSAFE now available on STN Easy
NEWS 12 NOV 26 Two new SET commands increase convenience of STN
                searching
NEWS 13 DEC 01
                ChemPort single article sales feature unavailable
NEWS 14 DEC 12 GBFULL now offers single source for full-text
                coverage of complete UK patent families
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NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 08:48:52 ON 16 DEC 2008

=> file reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 08:49:00 ON 16 DEC 2008
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STRUCTURE FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0 DICTIONARY FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

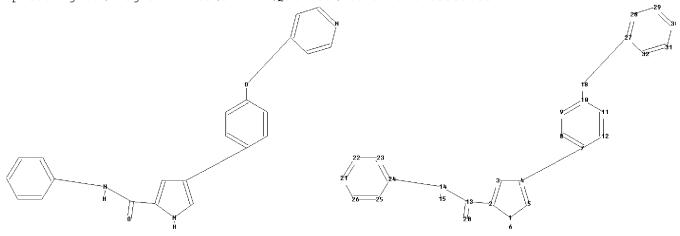
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\STNEXP\Queries\10579825 elected.str



chain nodes :

6 13 14 15 18 20

ring nodes :

 $\begin{smallmatrix} 1 & 2 & 3 & 4 & 5 & 7 & 8 & 9 & 10 & 11 & 12 & 21 & 22 & 23 & 24 & 25 & 26 & 27 & 28 & 29 & 30 & 31 & 32 \end{smallmatrix}$

chain bonds :

1-6 2-13 4-7 10-18 13-14 13-20 14-15 14-24 18-27

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 21-22 21-26 22-23 23-24 24-25 25-26 27-28 27-32 28-29 29-30 30-31 31-32

exact/norm bonds:
1-2 1-5 10-18 13-14 13-20 14-24 18-27
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normalized bonds:
7-8 7-12 8-9 9-10 10-11 11-12 21-22 21-26 22-23 23-24 24-25 25-26 27-28
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isolated ring systems:
containing 1: 7: 21: 27:

G1:0,S,N

G2:Cb,Cy,Hy

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 18:CLASS 20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:CLASS 31:CLASS 32:Atom

L1 STRUCTURE UPLOADED

=> d L1 L1 HAS NO ANSWERS L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
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0.67

FILE 'CAPLUS' ENTERED AT 08:49:17 ON 16 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25 FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

Caplus now includes complete International Patent Classification (IPC)

reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l1 SSS Full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 08:49:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 417 TO ITERATE

100.0% PROCESSED 417 ITERATIONS

SEARCH TIME: 00.00.01

L2 4 SEA SSS FUL L1

L3 1 L2

=> d ibib abs hitstr 1-YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:469894 CAPLUS Full-text

DOCUMENT NUMBER: 143:7592

TITLE: Preparation of arylpyrrolecarboxamides as Raf kinase

inhibitors for treatment of tumors.

INVENTOR(S): Finsinger, Dirk; Buchstaller, Hans-Peter; Burgdorf,

Lars; Wiesner, Matthias; Amendt, Christiane; Grell,

4 ANSWERS

Matthias; Sirrenberg, Christian; Zenke, Frank

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany

SOURCE: Ger. Offen., 32 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE			
DE 10354060	A1 20050602		20031119			
AU 2004291255 CA 2546334	A1 20050602 A1 20050602	CA 2004-2546334	20041026 20041026			
WO 2005049603 W: AE, AG, AL,	A1 20050602 , AM, AT, AU, AZ,	2 WO 2004-EP12076 BA, BB, BG, BR, BW, BY,	20041026 BZ, CA, CH,			
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                                          DE 2003-10354060 A 20031119
PRIORITY APPLN. INFO.:
                                          WO 2004-EP12076 W 20041026
OTHER SOURCE(S):
                       MARPAT 143:7592
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GT

AB Title compds. [I; Ar = (substituted) Ph, naphthyl, biphenyl, heterocyclyl; X = O, S, (CH2)n, CO, (CH2)nO, (CH2)nNH, etc.; n = 1-3; Y = O, S, CHNO2, C(CN)2, NR4; R4 = H, cyano, OH, etc.; Z = Ar, ArXAr, CH2Ar, CH2ArXAr; Ar = (substituted) Ph], were prepared as Raf kinase inhibitors (no data). Thus, 4-(PhCH2O)C6H4CH2CO2H, DMF, and POCl3 were heated together at $70\,^{\circ}$ for 4 h followed by cooling and addition of ice water and aqueous NaClO4 to give 98% [2-(4-benzyloxyphenyl)-3-dimethylaminoallylidene]dimethylammonium perchlorate. This was refluxed 24 h with glycine Et ester hydrochloride in EtOH containing 20% NaOEt to give 91% Et 4-(4-benzyloxyphenyl)-1H-pyrrole-2-carboxylate. Hydrogenolysis of the latter in EtOAc over Pd/C gave 91% Et 4-(4hydroxyphenyl)-1H-pyrrole-2-carboxylate. This was heated with 4chloropyridine-2-carboxylic acid N-methylamide at 160° for 48 h to give 40% Et 4-[4-(2-methylcarbamovlpyridin-4-yloxy)phenyl]-1H-pyrrole-2- carboxylate. Saponification with 2N NaOH in EtOH at 60° for 16 h followed by acidification with HCl gave 85% free acid, which was stirred 48 h in DMF with 5-amino-2chlorobenzotrifluoride, N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride, and 1-hydroxybenzotriazole hydrate to give 17% 4-[4-[5-(4chloro-3-trifluoromethylphenylcarbamoyl)-1H-pyrrol-3- yl]phenoxy]pyridine-2carboxylic acid N-methylamide.

ΙT 852455-19-7P 852455-21-1P 852455-22-2P 852455-24-4P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of arylpyrrolecarboxamides as Raf kinase inhibitors for treatment of tumors)

852455-19-7 CAPLUS RN

CN 2-Pyridinecarboxamide, 4-[4-[5-[[[4-chloro-3(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl-(CA INDEX NAME)

RN 852455-21-1 CAPLUS

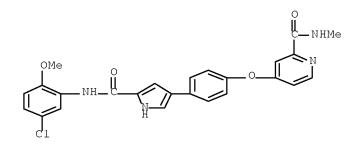
CN 2-Pyridinecarboxamide, 4-[4-[5-[[(3-chloro-4-methylphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)

RN 852455-22-2 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[5-[[[2-methoxy-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl-(CA INDEX NAME)

RN 852455-24-4 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[5-[[(5-chloro-2-methoxyphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



=> file marpat

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
6.89
186.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE -0.80 -0.80

FILE 'MARPAT' ENTERED AT 08:51:09 ON 16 DEC 2008
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FILE CONTENT: 1961-PRESENT VOL 149 ISS 24 (20081212/ED)

MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 20080280867 13 NOV 2008 DE 102008019744 30 OCT 2008 ΕP 1990054 12 NOV 2008 JΡ 2008262895 30 OCT 2008 WO 2008136863 13 NOV 2008 2448808 29 OCT 2008 GB 2915685 07 NOV 2008 FR 2337918 10 NOV 2008 RU CA 2629177 18 OCT 2008

Expanded G-group definition display now available.

The new MARPAT User Guide is now available at: http://www.cas.org/support/stngen/stndoc/marpat.html.

=> s L1 SSS Full

FULL SEARCH INITIATED 08:51:13 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 8419 TO ITERATE

100.0% PROCESSED 8419 ITERATIONS SEARCH TIME: 00.00.07

3 ANSWERS

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 125.26 311.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -0.80

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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25 FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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http://www.cas.org/legal/infopolicy.html

=> s L4

L5 3 L4

=> d ibib abs hitstr 1-YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:469894 CAPLUS Full-text

DOCUMENT NUMBER: 143:7592

TITLE: Preparation of arylpyrrolecarboxamides as Raf kinase

inhibitors for treatment of tumors.

INVENTOR(S): Finsinger, Dirk; Buchstaller, Hans-Peter; Burgdorf,

Lars; Wiesner, Matthias; Amendt, Christiane; Grell,

Matthias; Sirrenberg, Christian; Zenke, Frank

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany

SOURCE: Ger. Offen., 32 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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OTHER SO	THER SOURCE(S):					MARPAT 143:7592													

XAr

GΙ

Title compds. [I; Ar = (substituted) Ph, naphthyl, biphenyl, heterocyclyl; X = O, S, (CH2)n, CO, (CH2)nO, (CH2)nNH, etc.; n = 1-3; Y = O, S, CHNO2, C(CN)2, NR4; R4 = H, cyano, OH, etc.; Z = Ar, ArXAr, CH2Ar, CH2ArXAr; Ar = (substituted) Ph], were prepared as Raf kinase inhibitors (no data). Thus, 4-

(PhCH2O)C6H4CH2CO2H, DMF, and POCl3 were heated together at 70° for 4 h followed by cooling and addition of ice water and aqueous NaClO4 to give 98%

[2-(4-benzyloxyphenyl)-3-dimethylaminoallylidene]dimethylammonium perchlorate. This was refluxed 24 h with glycine Et ester hydrochloride in EtOH containing 20% NaOEt to give 91% Et 4-(4-benzyloxyphenyl)-1H-pyrrole-2-carboxylate. Hydrogenolysis of the latter in EtOAc over Pd/C gave 91% Et 4-(4-hydroxyphenyl)-1H-pyrrole-2-carboxylate. This was heated with 4-chloropyridine-2-carboxylic acid N-methylamide at 160° for 48 h to give 40% Et 4-[4-(2-methylcarbamoylpyridin-4-yloxy)phenyl]-1H-pyrrole-2- carboxylate. Saponification with 2N NaOH in EtOH at 60° for 16 h followed by acidification with HCl gave 85% free acid, which was stirred 48 h in DMF with 5-amino-2-

chlorobenzotrifluoride, N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride, and 1-hydroxybenzotriazole hydrate to give 17% 4-[4-[5-(4chloro-3-trifluoromethylphenylcarbamoyl)-1H-pyrrol-3- yl]phenoxy]pyridine-2carboxylic acid N-methylamide.

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:14213 CAPLUS Full-text

DOCUMENT NUMBER: 142:114071

TITLE: Preparation of substituted 5-membered ring compounds

as heat shock protein 90 (HSP90) inhibitors

Cheung, Kwai Ming; Dymock, Brian William; MacDonald, INVENTOR(S):

Edward; Drysdale, Martin James

PATENT ASSIGNEE(S): Vernalis Cambridge Limited, UK; Cancer Research

Technology Ltd.; The Institute of Cancer Research

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

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OTHER S	OURCE	(S):			MAR	PAT	142:	1140	71								

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AB Title compds. I [wherein A = 5-membered cycle; R1 = (un)substituted (hetero)aryl; R2 (adjacent to R1) = absence, H, carboxamide, (un)substituted (hetero)aryl, carbocycle or heterocycle; R3 (adjacent to R2) = absence, H, (un)substituted cycloalky(en)yl, alk(en/yn)yl, carboxyl, carboxamide or ester; with some limitations, or salts, N-oxides, hydrates or solvates thereof] were prepared as heat shock protein 90 (HSP90) inhibitors. Thus, 5-chloro-2,4-dimethoxyphenylamine was treated with NaNO2 in the presence of H2SO4 followed by the addition of NaN3. The resultant azide underwent cyclization with 3-(4-fluorophenyl)-3-oxopropionic acid Me ester gave intermediate II (X = OMe, R= OH). Demethylation of this compound with 48% HBr followed by esterification with EtOH yielded triazolecarboxylate II (X = OH, R = OEt), which showed IC50 <10 μM for binding to HSP90 in a fluorescence polarization assay. Therefore, I and their compns. are useful for immunosuppression or the treatment of cancers, viral disease, inflammatory diseases and so on.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:589375 CAPLUS Full-text

DOCUMENT NUMBER: 141:140459

TITLE: Preparation of sulfamides as anti-cancer agents

INVENTOR(S): Flynn, Daniel L.; Petrillo, Peter A. PATENT ASSIGNEE(S): Deciphera Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 168 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

					KIND DATE			APPLICATION NO.											
								WO 2003-US41425											
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		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	KΖ,	LC,	LK,	LR,		
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		TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	ΤG	
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OTHER SOURCE(S): MARPAT 141:140459

AB Sulfamides, such as I, were prepared for use as anticancer agents which act by modulating the activation states of abl or bcr-abl α -kinase proteins. Thus, 4-HO2CC6H4CH2NHSO2NHCOR [R = pyrrolidino], prepared from 4-MeO2CC6H4CH2NH2 and pyrrolidine, was treated with the pyrimidinylaminoaniline fragment to give I, which showed 10% inhibition of non-phosphorylated abl kinase at 10 μ M.

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